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**EVALUATION OF THE HEAT TRANSFER MODULE (FAHT) OF FAILURE
ANALYSIS NONLINEAR THERMAL AND STRUCTURAL INTEGRATED
CODE (FANTASTIC)**

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Evaluation of the Heat Transfer Module (FAHT) of Failure Analysis Nonlinear
Thermal and Structural Integrated
Code (FANTASTIC)

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ABSTRACT

The heat transfer module of FANTASTIC Code (FAHT) is studied and evaluated to the extend possible during the ten weeks duration of this project. A brief background of the previous studies is given and the governing equations as modeled in FAHT are discussed. FAHT's capabilities and limitations based on these equations and its coding methodology are explained in detail. It is established that with improper choice of element size and time step FAHT's temperature field prediction at some nodes will be below the initial condition. The source of this unrealistic temperature prediction is identified and a procedure is proposed for avoiding this phenomenon. It is further shown that the proposed procedure will converge to an accurate prediction upon mesh refinement. Unfortunately due to lack of time, FAHT's ability to accurately account for pyrolysis and surface ablation has not been verified. Therefore, at the present time it can be stated with confidence that FAHT can accurately predict the temperature field for a transient multi-dimensional, orthotropic material with directional dependence, variable property, with nonlinear boundary condition. Such a prediction will provide an upper limit for the temperature field in an ablating decomposing nozzle liner. The pore pressure field, however, will not be known.

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NOMENCLATURE

| | |
|------------|--|
| B | Permeability matrix |
| B_{ij} | Components of the Permeability matrix |
| C_m | Defined by Eq. (FAHT-5) |
| C_p | Specific heat |
| k | Thermal Conductivity |
| K | Thermal Conductivity matrix |
| K_{ij} | Components of the Thermal Conductivity matrix |
| P | Pore pressure |
| Q | Volumetric heat source/sink |
| Q_c | Heat convected by pyrolysis gas, defined by Eq. (FAHT-2) |
| R_g | Specific gas constant |
| \dot{S} | Rate of surface recession |
| t | Time |
| Δt | Time step size in an analysis |
| T | Temperature |
| T_g | Gas Temperature |
| T_i | Initial Temperature |
| T_s | Surface Temperature |
| V | Velocity vector |
| ∇ | Vector differential operator del |
| x | Coordinate in 3-D space |
| x_i | A generic cartesian coordinate |
| Δx | Element thickness in the direction of heat flow |
| α | Thermal diffusivity |
| δ | Penetration depth |
| γ | Defined by Eq. (FAHT-3) |
| ϵ | Emissivity |
| λ | Eigen value of the exact solution |
| μ | Dynamic viscosity |
| n | Pi |
| ρ | Density |
| ϕ | Porosity |
| Φ | Volumetric mass source/sink |

I. INTRODUCTION

I.1 Overview

The FANTASTIC code is in its final stage of development by Failure Analysis Associates (FaAA) for Marshall Space Flight Center. The code is presently under review and evaluation for its capabilities. The intended use of the Code is to increase the capabilities and accuracy of the thermal and structural analysis of solid rocket motor nozzles. The code consists of three modules for thermochemical analysis, heat transfer and mass diffusion analysis, and structural analysis.

II.2 Objectives of the Present Work

The present work is limited to the evaluation of the heat transfer and mass diffusion module (FAHT) of the FANTASTIC Code. In order to proceed with the stated task within the rather short time period of the project, the following sub-tasks were chosen:

1. A brief review of previous efforts in the area of code development.
2. Verification of the various required capabilities of the FAHT module, such as transient, nonlinear boundary condition and variable property solution routines.
3. A limited attempt at use of FAHT for prediction of the temperature distribution in MNASA nozzle.

II. BACKGROUND

Charring ablators have proven to be one of the most successful thermal protection systems for applications with high thermal loading such as reentry and solid rocket nozzles. The materials used are a combination of plastics that decompose to a porous char zone and pyrolysis gases. The pyrolysis gases transport energy to the surface under thermal loading thereby reduce the rate of energy input into the virgin material. The decomposition process along with endothermic reactions of the pyrolysis gases with the carbon in the char zone are of further help in reducing the rate of energy input into the virgin material. A cross-sectional view of a charring and decomposing ablator of a nozzle is depicted in Fig. 1. The events taking place in the char and pyrolysis zones can be summarized as follows:

Char Zone

- a. Thickness of this zone is about 2 to 4 mm depending on the material used.
- b. Pyrolysis gases flowing through this porous zone have a cooling effect due to convective transport of energy to the surface.
- c. Pyrolysis gases are not frozen in this region and endothermic reactions with carbon of the char zone takes place, resulting in a "cooling" of the char zone.
- d. Chemical reactions between the char zone and the pyrolysis gases result in a constant change in the porosity and the permeability of the char layer.

Pyrolysis Zone

- a. Thickness of this zone in typical ablators is about 1 to 2 mm.
- b. Porosity and permeability in this region are changing rapidly.
- c. A volumetric energy source/sink is present due to decomposition of the virgin material.

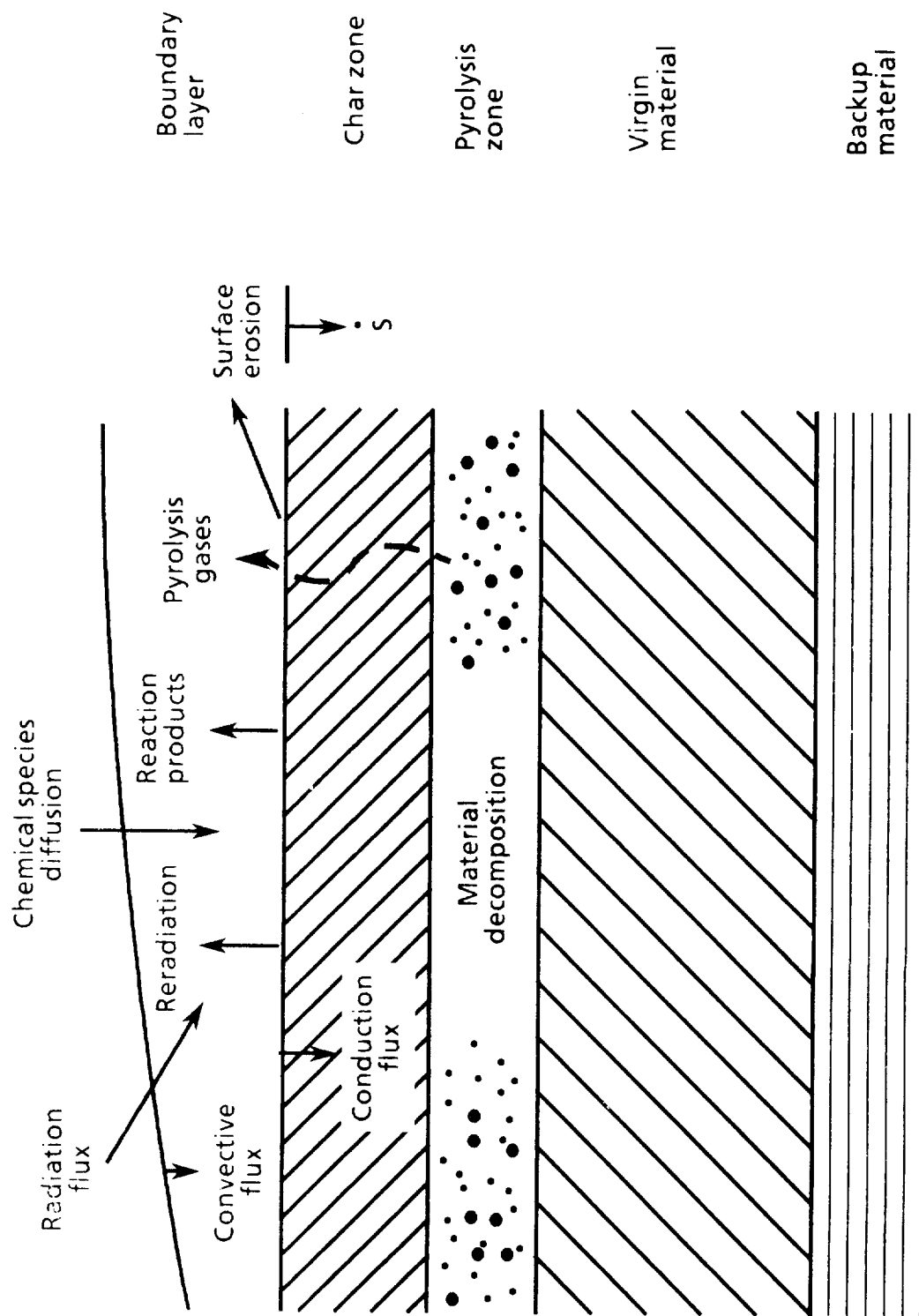


Figure 1. Cross-sectional view of a charring and decomposing ablator of a nozzle.

The above summary of the phenomena taking place in a charring ablator clearly shows the complexity of the problem. Other factors that add to the difficulty of accurate prediction of temperature and pore pressure values in a charring ablator are:

- a. Temperature variation in space and time is substantial, therefore the evaluation of the thermophysical properties at the proper temperature is very important.
- b. The material is orthotropic, therefore the conservation equations for energy and momentum are more difficult to model.
- c. As mentioned earlier porosity and permeability are changing with time. Therefore, they are variables in the momentum equation. The porosity variation can be accounted for via its relation to density variation governed by the rate equation of the Arrhenius form. The modeling of the variable permeability for an orthotropic material, however, is not trivial. It appears that no empirical relation for relating the permeability of this class of materials to its porosity is available at the present time.
- d. The nonequilibrium chemical reaction between the pyrolysis gases and the char zone has not been thoroughly investigated for all the candidate materials for nozzle liner.

II.1 Previous Work

A review of the literature indicates that research and code development effort in the area of thermal analysis of charring and decomposing ablators had a rather high priority for NASA during the decade of 1962-1972. It appears that the development of new candidate materials for a charring-decomposing ablator may require initiation of a rigorous research program in this important area. A brief summary of the previous work is given in this report.

- Aerotherm charring material thermal response and ablation program (CMA, Aerotherm report 75-148, 1975)
 - One-dimensional transient finite difference model
 - No resistance to flow of pyrolysis gases
 - Frozen flow of pyrolysis gases through the char zone
- NASA report NASA TN-D-6895 (1972)
 - Two-dimensional transient axisymmetric finite difference model
 - Resistance to flow of pyrolysis gases incorporated via Darcy's law
 - Frozen flow of pyrolysis gases through char zone
- NASA reports NASA TN D-1370 (1962) CHAP I and NASA TN D-2976 (1965) CHAP II
 - One-dimensional Transient finite difference program
 - No resistance to flow of pyrolysis gases
 - Frozen Flow of Pyrolysis gases through the char zone (CHAP I)
 - Chemical reaction between the pyrolysis gases and the char incorporated (CHAP II)
- NASA report NASA TN D-6085 (1970), COSMIC
 - One dimensional transient finite difference model
 - No resistance to flow of pyrolysis gases
 - Frozen flow of pyrolysis gases through the char zone

- NASA report NASA CR-1903 (1971)
 - One-dimensional steady-state finite difference model
 - Modified form of Darcy's equation used to model resistance to flow of pyrolysis gases
 - Flow of pyrolysis gases through the char zone analyzed as
 1. Frozen
 2. Equilibrium
 3. Non-Equilibrium

II.2 Governing Equations

In this section the energy, momentum and mass conservation equations as they appear in the FANTASTIC/FAHT theoretical manual (version 1.0) will be reported and discussed.

Energy equation:

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial T}{\partial x_j} \right) + Q \quad (\text{FAHT-1})$$

The volumetric source/sink term (Q) in Eq. (FAHT-1) accounts for the energy associate with the decomposition process. It should be noted that the energy transport term due to convection of pyrolysis gases does not appear in Eq. (FAHT-1). FAHT theoretical manual states that the heat convected by pyrolysis gases is calculated by

$$Q_c = \rho C_p \mathbf{V} \cdot \nabla T, \quad (\text{FAHT-2})$$

and can be accounted for via: NONLINEARHEATBC, THERMALGAPCONTACT OR LUMPEDHEATCAPACITY Options.

Proper form of the energy equation is given by

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{V} \cdot \nabla T = \frac{\partial}{\partial x_i} \left(K_{ij} \frac{\partial T}{\partial x_j} \right) + Q \quad (1)$$

It is very important to note that the temperature pressure and velocity in a decomposing ablator are undergoing substantial changes with a rather small change in time. Literature contains a very large volume of papers dealing with various convection heat transfer problems. This author is not aware of a single case where the convection term is not explicitly treated in the energy equation as is the case with Eq. (FAHT-1).

In verbal communication with Dr. McCoy (NASA/MSFC-ED64) FaAA Personnel have stated that the heat convected by pyrolysis gases (Eq. FAHT-2) is accounted for as part of the load term Q. In that case the energy equation is not related accurately.

Momentum Equation:

$$\mathbf{V} = - \frac{\gamma}{\phi \mu} \mathbf{B} \nabla P^T \quad (\text{FAHT-3})$$

$$\gamma = R_g \text{ when ideal gas or } \gamma = \frac{dP}{d\rho}$$

The momentum equation as given by Eq. (FAHT-3) is dimensionally inconsistent. The proper form of the momentum equation based on the Darcy law is

$$\mathbf{V} = - \frac{1}{\phi \mu} \mathbf{B} \cdot (\nabla P) \quad (2)$$

Mass Conservation Equation:

$$\frac{d}{dt} [\phi \rho] + \nabla \cdot (\phi \rho \mathbf{V}) = \Phi \quad (\text{FAHT-4})$$

In order to obtain an explicit equation for pore pressure, FAHT theoretical manual states that Eqs. (FAHT-3) and (FAHT-4) are combined to get,

$$\frac{\partial}{\partial t} [C_m P] = \frac{\partial}{\partial x_i} \left(\frac{B_{ij}}{\mu} \frac{\partial P}{\partial x_j} \right) + \Phi \quad (\text{FAHT-5})$$

$$\text{where } C_m = \phi \frac{\partial \rho}{\partial P} \quad \text{or} = \quad \frac{\phi}{R_g T}$$

It should be noted that the pore pressure equation as given by Eq. (FAHT-5) is also dimensionally inconsistent. The proper form of the pore pressure equation is

$$\frac{d}{dt} (\phi \rho) = \frac{\partial}{\partial x_i} \left(\frac{\rho B_{ij}}{\mu} \frac{\partial P}{\partial x_j} \right) + \Phi \quad (3)$$

$$\text{where } \rho = \frac{P}{R_g T}$$

The problem with Eqs. (FAHT-3) and (FAHT-5) may be due to a typographical error, and they are correct in the program. If that is the case, then it is an indication of a poor editing job of various versions of manual up to version 1.0 which have been released by FaAA.

II.3 FAHT'S Capabilities and Limitations

In order to get an estimate of FAHT's potential capabilities it is necessary to come to a conclusion about the governing equations as described in FAHT's theoretical manual (version 1.0). The following assumptions are made with regards to modeling of the governing equations in the FAHT module.

- (a) The convected energy by the pyrolysis gases are accounted for as part of the load term (Q) in Eq. (FAHT-1)
- (b) The problem with Eqs. (FAHT-3) and (FAHT-5) is typographical, and these equations are indeed dimensionally consistent in the program.

Based on the above assumptions, FAHT's potential capabilities in analysis of a charring-decomposing ablator are as follows:

- (i) The temperature field solution will have some errors due to lack of explicit treatment of the convection term.
- (ii) The pore pressure equation, as given by Eq. (3) is nonlinear. This equation, however, is treated as a linear equation in FAHT. Therefore, the pore pressure solution will not be accurate, which will result in an inaccurate velocity solution. The inaccuracy associated with the velocity solution, in turn, will increase the error in the temperature solution.
- (iii) The flow of pyrolysis gases through the char zone are modeled as a non-reacting low (frozen). Therefore, the endothermic reactions which take place in this zone can not be accounted for. Furthermore, the changes in the porosity and permeability in this zone cannot be calculated and accounted for.
- (iv) The permeability of the material is assumed to have the same value in the virgin, decomposition and char zones. As mentioned earlier, the permeability is changing rapidly with time in the decomposition zone. Nonetheless, FAHT can not account for this variation.
- (v) There are no provisions for accounting for the initial porosity of the virgin material.
- (vi) The momentum equation is based on the Darcy law. However, it is known (NASA CR-1903, 1971) that the inertial effects play an important role due to relatively high mass fluxes of the degradation products. An accurate modeling of the momentum equation requires the inclusion of the Forchheimer term. Another motivation for the use of Forchheimer-extended Darcy equation of motion for flow through porous media is the following. One of the objectives of the exploratory test program of the Solid Propulsion Integrity Program (SPIP) is to provide empirical relations for permeability of various candidate materials. There may be cases where the permeability should be determined via the Forchheimer-extended Darcy equation. In that case we do not have any analysis tool that can properly use the permeability data.

III. VERIFICATION OF FAHTS' CAPABILITIES

III.1 Transient Solution Routine

In the process of assessment and verification of the heat transfer module of the FANTASTIC code, many attempts have been made at obtaining solutions for simple cases of transient conduction heat transfer. It appears that in many cases the predicted short-time temperatures at some nodes were below the initial input values. Thus, the code indicated that those nodes were cooling while the physics of the problem imposed a rather high heating rate for the material. A number of explanations along with corrective remedies have been forwarded by FaAA. It has been suggested by FaAA that for high heating rate cases (high thermal gradients) the input values of time step and element size should be such that the value of the element Fourier number is rather low. The element Fourier number is defined as $\alpha \Delta t / \Delta x^2$. The parameter α is the thermal diffusivity of the material and can not be arbitrary changed. The only alternative for reducing the element Fourier number is then using a smaller time step and/or larger elements. The choice of a smaller time step and/or larger element size does not resolved the problem and indeed results in even lower values. Therefore, we are in a situation where we cannot get realistic solutions to transient problems with high heating rates. It may be noted that our intended application is precisely what FAHT apparently cannot solve.

The source of the problem with the FAHT's inability for solving transient problems with high gradients is not a "bug." It is a rather fundamental problem related to the physics of the process. Before we proceed further, the terms "unrealistic" and "realistic" should be defined. First, note that in solving "real world" problems we do not know the exact answer. Thus, a realistic answer is one which makes physical sense to the analyst but may not be accurate. Realistic answers can be very dangerous. Shortly, I will explain why I consider them dangerous to an inexperienced analyst. The unrealistic answer is very easy to detect such as the case of cooling nodes predicted by FAHT where the model has specified a high heating rate.

Finite difference computer codes rarely give an unrealistic answer to a high heating rate transient problem. However, finite element codes, depending on the choice of

shape function, are prone to give unrealistic answers when the thermal gradients are high. As stated earlier, the problem with this class of finite element programs (including FAHT) is one of fundamental nature. A high thermal gradient results in a propagation of a thermal front into an isothermal domain (initial condition). For a given time step, this thermal front moves into the domain by a distance called penetration depth (δ). Figure 2 depicts the movement of penetration depth into a domain. If δ is smaller than the element length (Δx), then depending on the choice of the shape function, the nodal temperatures are determined with unrealistic values as depicted in Fig. 3. For further detail about this phenomena please refer to Hogge and Gerrekens (1982). The remedy for this problem is a choice of a larger time step and/or smaller elements. Obviously, if the solution routine is explicit, then the chosen time step should not violate the stability criterion.

To illustrate the fact that the suggested remedy does indeed result in a realistic answer by FAHT, let's consider a simple test problem as shown in Fig. 4.

Test Problem

Transient one-dimensional conduction heat transfer
in a plane wall with constant properties. The
parameters of the problem are:

width of the wall = 0.2m

density = 2600 kg/m³

specific heat = 808 J/kg·K

thermal conductivity = 3.98 W/m·K

Boundary Conditions:

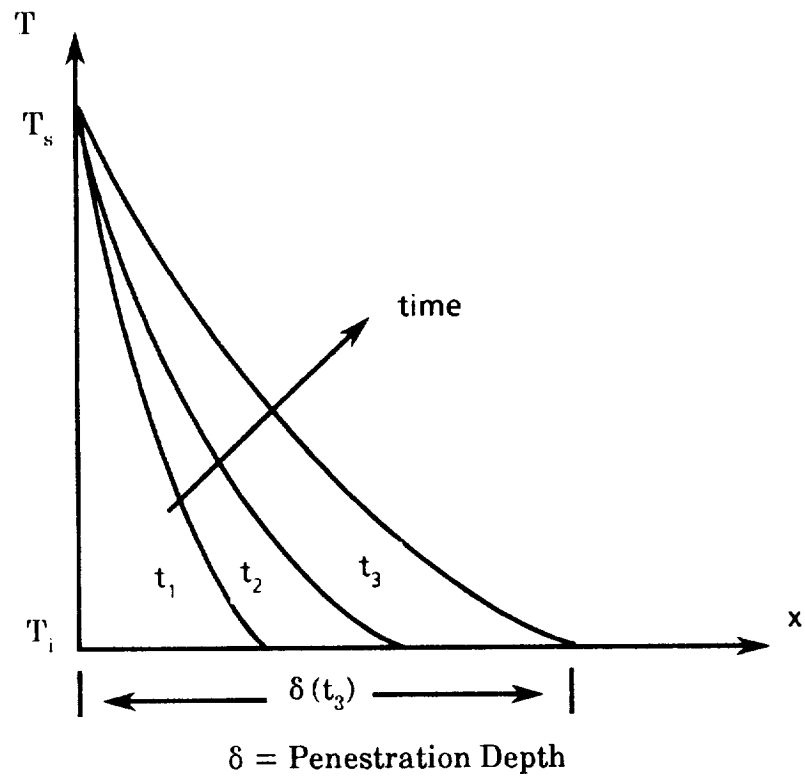
$T(x = 0, t) = T_s = 3600 \text{ K}$

$\partial T / \partial X (x = L, t)$, insulated backwall

Initial Condition:

$T(x, t = 0) = T_i = 300 \text{ K}$

The temperature distribution in the wall at time = 10 seconds will be presented in the following tables. All solutions are obtained via the implicit formulation.



$$T(0,t) = T_s; \quad \left. \frac{\partial T}{\partial x} \right|_{x=\infty} = 0;$$

$$T(x,0) = T_i$$

Figure 2. Short-time transient temperature profile in a domain.

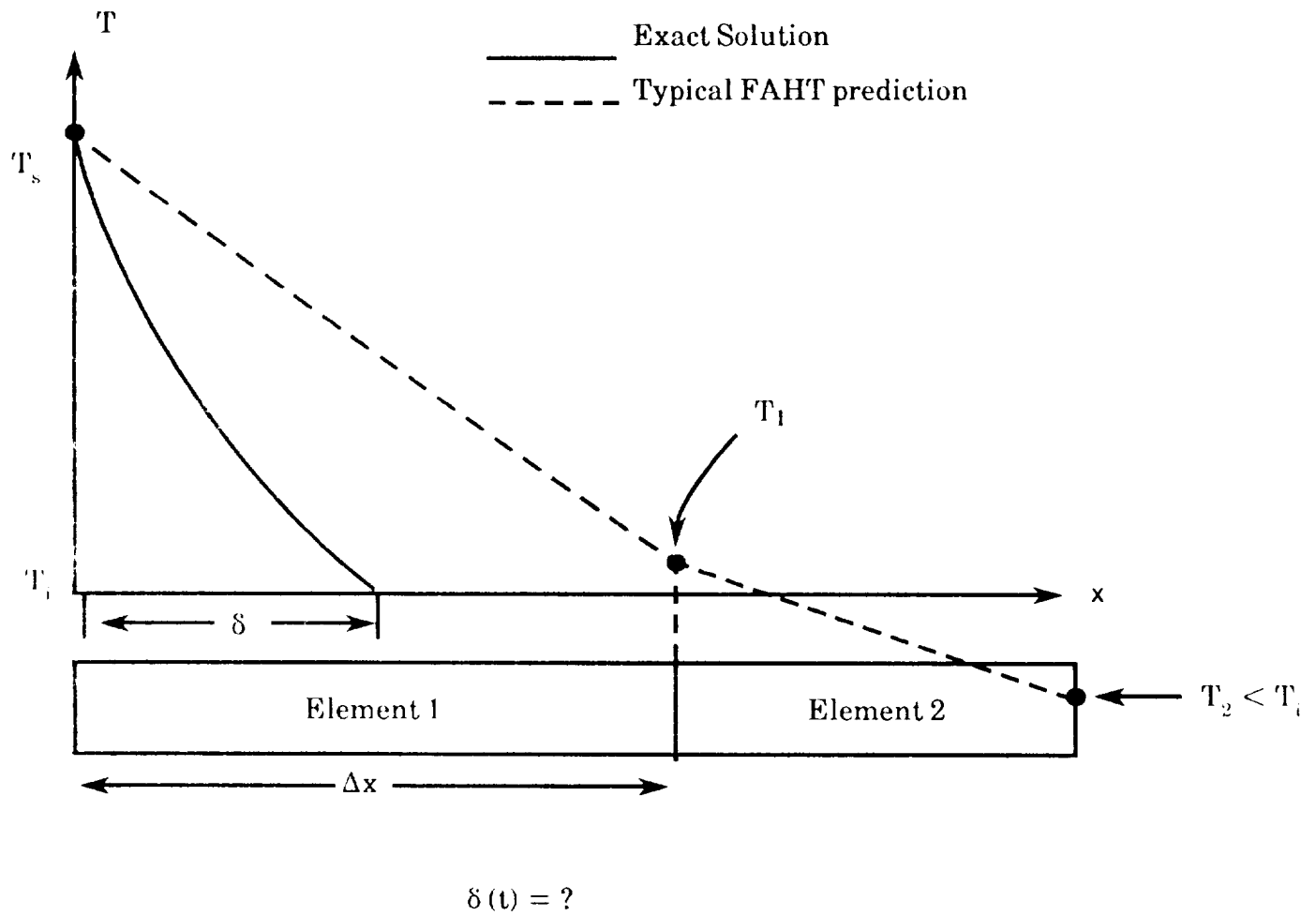
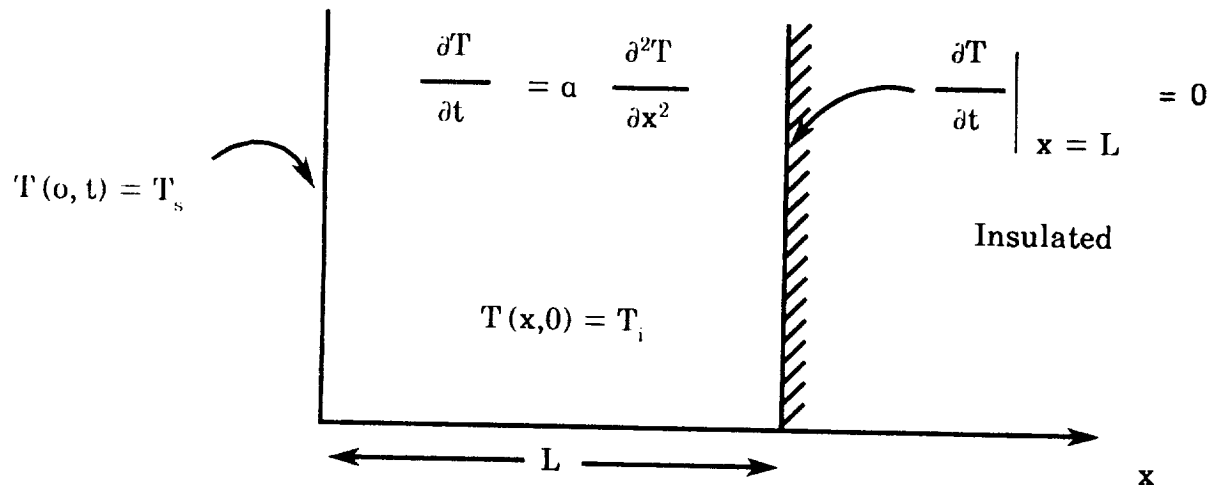


Figure 3. Element size (Δx) versus Penetration depth (δ).



Input Data:

$$T_s = 3600 \text{ K}, \quad T_i = 300 \text{ K}$$

$$K = 3.98 \text{ W/m}\cdot\text{K}$$

$$\rho = 2600 \text{ Kg/m}^3$$

$$C_p = 808 \text{ J/Kg}\cdot\text{K}$$

$$L = 0.2 \text{ m}$$

Exact Solution:

$$\frac{T(x, t) - T_i}{T_s - T_i} = 1 - \frac{4}{\pi} \sum_{n=0}^{\infty} \frac{\sin(\lambda_n x)}{(2n+1)} e^{-(\lambda_n^2 \alpha t)}$$

$$\lambda_n = \frac{(2n+1)\pi}{2L}$$

Figure 4. Description of the test problem and its exact solution.

Table 1: FAHT temperature predictions ($T(x,t) - T_i$) for various element sizes, and time steps at time = 10 seconds.

| Run No. | $X = 0.01$ (m) | 0.02 | 0.03 | 0.04 | No. of Elements | Time Step (Seconds) |
|---------|----------------|--------|------|------|-----------------|---------------------|
| FE-1 | 189.4 | -120.1 | 24.6 | -2.4 | 20 | 2 |
| FE-2 | 261.1 | -124.3 | 20.3 | -0.4 | 20 | 0.2 |
| FE-3 | 233.0 | -6.9 | -0.1 | 0.03 | 40 | 2 |
| FE-4 | 272 | 1.0 | 0 | 0 | 80 | 2 |

The following observations can be made with regards to the results in Table 1:

- A comparison of the results of runs FE-1 and FE-2 shows that when unrealistic (negative) nodal values are obtained, a decrease in time step does not help.
- A comparison of the results of runs FE-1, FE-3, and FE-4 indicates that when unrealistic nodal values are obtained, increasing the number of elements thereby decreasing Δx yields a realistic solution.
- Consider that the exact answer is unknown. Furthermore, consider that the first choice of an analyst was the input values of run FE-4. The results of this run are indeed realistic and make sense. A 20cm wall is divided into 80 elements ($\Delta x = 2.5$ mm). Moreover, a time step of 2 seconds for transition from zero time to 10 seconds is rather a reasonable choice.
- The above discussion indicates that the analyst may well choose to accept the results of run FE-4 as reasonable. However, the "realistic" answer of the run FE-4 is in substantial error. Indeed, the values at $x = 0.01$ and 0.02 are, respectively, 21% and 74% lower than the exact answer. This is a good example of the case where "realistic" answers should be treated with caution.

I hope that my earlier comment about the potential danger of a “realistic” answer is clarified. It is reasonable to ask then, how should an analyst ensure that the realistic answer is reasonably accurate when the accurate answer is unknown?

The penetration depth (δ) of a thermal front into an isothermal semi-infinite domain can be approximated as (Ozisik, 1980)

$$\delta \approx \sqrt{12 \alpha t} \quad (4)$$

In order to obtain a realistic answer, δ for the first time step should be large enough to cover a number of elements i.e.,

$$\delta(\Delta t) = \sqrt{12 \alpha \Delta t} > \Delta x \quad (5)$$

The stability criterion for the explicit solution scheme is given by,

$$\Delta x > \sqrt{2 \alpha \Delta t} \quad (6)$$

Equation (6) describes an inter-dependence between the time step and the element size. In implicit solution routines this equation is irrelevant in terms of the stability. However, any stable implicit solution is not necessarily an accurate solution. In order to ensure that an implicit solution is a fairly accurate one, gross violations of equation (6) should be avoided.

The following relation which satisfies equation (5) and does not result in a gross violation of equation (6) is proposed

$$\sqrt{\alpha \Delta t} < \Delta x < \sqrt{3 \alpha \Delta t} \quad (7)$$

The upper limit in the equation (7) ensures that δ for the first time step covers more than two elements. The lower limit on Δx as given by equation (6) is relaxed by a factor of $\sqrt{2}$.

A Suggested Procedure for Obtaining Accurate Transient Results from FAHT:

1. Start with a reasonable time step.
2. Select Δx by calculating the acceptable limits, and obtain the code prediction.

$$\sqrt{\alpha \Delta t} < \Delta x < \sqrt{3 \alpha \Delta t} \quad (8)$$

3. Reduce Δx by a factor of two and select Δt using the following relation, and obtain the solution for the new Δx and Δt .

$$\frac{\Delta x^2}{3\alpha} < \Delta t < \frac{\Delta x^2}{\alpha} \quad (9)$$

4. Compare the two results. If the changes in the temperature field are more than an "acceptable variation" then repeat step 3. Obviously, the degree of the accuracy depends on the selected criterion for the "acceptable variation."

It should be noted that the above procedure for selection of Δt violates the stability criterion for explicit scheme and should not be used for explicit solution.

Let's apply the above procedure to the example problem:

Step 1: $\Delta t = 2$ seconds (the same as run FE-1).

Step 2: $1.95\text{mm} < \Delta x < 3.37\text{mm}$. Select $\Delta x = 2.5\text{mm}$ (80 elements). This step clearly shows that for a time step of $\Delta t = 2$ seconds, 20 and 40 elements runs were inappropriate. Note that the results for $\Delta x = 2.5\text{ mm}$ and $\Delta t = 2\text{ sec.}$ are realistic (please see Table 2).

Step 3: Double the number of elements.
160 elements; $\Delta x = 1.25\text{ mm}$.
 $0.27 < \Delta t < 0.82$; choose $\Delta t = 0.4$ seconds.

Step 4: A substantial change in the temperature field is observed. Repeat step 3.
320 elements; $\Delta x = 0.625\text{ mm}$.
 $0.07 < \Delta t < 0.21$; choose $\Delta t = 0.1$ seconds.

The results of these numerical experiments are tabulated in Table 2. The exact solution is also given in this table. A finite difference code based on the implicit formulation was programmed and the above outline for a "search" for an "accurate" answer was followed. The results of this program are also included in Table 2.

TABLE 2. "Search" for Accurate Temperature Prediction, $(T(x,t) - T_i)$, at Time = 10 seconds.

| Solution Method | $x = 0.01$ (m) | 0.02 | 0.03 | 0.04 | No. of Elements | Time Step (Seconds) |
|-------------------|-------------------|------|------|----------|-----------------|---------------------|
| Exact | 344.1 | 3.8 | 0.01 | ~ 0 | - | - |
| FAHT | | | | | | |
| FE-4 | 272 | 1.0 | 0 | 0 | 80 | 2 |
| FE-5 | 329.2 | 2.75 | 0 | 0 | 160 | 0.4 |
| FE-6 | 340.4 | 3.5 | 0 | 0 | 320 | 0.1 |
| Finite Difference | | | | | | |
| FD-1 | 352.6 | 14.2 | 2.0 | 0 | 80 | 2.0 |
| FD-2 | 345.6 | 6.1 | 0.03 | 0 | 160 | 0.4 |
| FD-3 | 344.4 | 4.4 | 0 | 0 | 320 | 0.1 |
| SINDA-87 | 344.9 | 4.4 | 0 | 0 | 320 | 0.1 |

The FAHT results in Table 2 show that the above procedure in 3 iterations resulted in a fairly accurate answer (compare runs FE-6 and FD-3 with the exact solution). The exact solution is given in Fig. 4.

A reflection on the number of elements or nodes used to obtain the results given in Table 2, points to the gross inefficiency in the grid selection. For example, 320 elements are uniformly distributed in the domain of $x = 0$ to 0.2. However, the results at time = 10 seconds show that the heat transfer is taking place in the region of $x = 0$ to 0.03, which contains 48 elements. Therefore, the remainder of the elements (272) are practically irrelevant. Of course, a number of techniques, such as deforming grid formulation, are available for efficient solution of this class of problems (Hogge and Gerrekens, 1982).

III.2 Nonlinear Boundary Condition Routine

In order to verify the nonlinear boundary condition routine of FAHT, the boundary condition of the test problem at the $x = 0$ surface is changed. There are various ways to impose a nonlinear boundary condition at this surface. The most logical one, considering the intended usage of the FAHT program, is a radiation boundary condition. Thus, the boundary condition at this surface is changed to radiation heat transfer from a gas at a temperature of $T_g = 3600$ K. The surface emissivity ϵ is taken to be 0.8. In section III.1 it was determined that for the test problem the values of $\Delta x = 0.625$ mm and $\Delta t = 0.1$ sec will result in an accurate solution by FAHT. Therefore, the radiation boundary condition problem is solved by FAHT with the same values for Δx and Δt . The predicted temperatures, $T(x,t) - T_i$, at time = 2 sec for nodes from $x = 0$ to 2.5 mm are tabulated in Table 3. In order to verify the accuracy of FAHT's prediction, the predicted values obtained from SINDA-87 program (for the same parameters) are also given in Table 3.

The maximum variation between the results of FAHT and SINDA-87 is less than 0.1%. It should be noted that SINDA-87 is a widely used program and its accuracy in solving rather complex problems has been established over the years. Therefore, it can be stated with confidence that FAHT's nonlinear boundary condition routine is reliable and accurate.

Table 3. Comparison of FAHT and Sinda-87 Temperature Predictions, $T(x,t) - T_i$, at Time = 2 seconds (Radiation Boundary Condition Verification).

| Code | $x = 0$ mm | 0.625 | 1.25 | 1.875 | 2.5 |
|----------|------------|-------|------|-------|------|
| FAHT | 3002 | 2410 | 1887 | 1448 | 1098 |
| SINDA-87 | 3001 | 2411 | 1888 | 1449 | 1099 |

- Test problem with $T_{gas} = 3600$ K, $\epsilon = 0.8$
- 320 elements, $\Delta t = 0.1$ sec
- Constant properties

III.3 Variable Property Routine

The radiation test case is extended to one with a variable thermal conductivity with $k = 3.98 + 0.002 T$, while density and specific heat are kept constant. The specified thermal conductivity function will result in an increase in k and thermal diffusivity by a factor 2.44 over the temperature range of 300 to 3600 K. It should be added that it is not necessary to have all the thermophysical properties as variables in order to verify the variable property routine. This is due to the fact that the same logic and routine is used to evaluate the new property values.

In section III.1 Eq. (9) was proposed for selection of a time step (for a given Δx) which would ensure a realistic answer, and upon further mesh refinement would lead to an accurate solution. Thermal diffusivity is a parameter in Eq. (9). For variable property problems, it is recommended to use the maximum and minimum values of α to obtain the corresponding limits on Δt . The maximum α value will result in a smaller allowable time step range. However, it should be noted that the thermal penetration front moves into the undisturbed domain at a temperature which is less than the maximum value. Once a region is penetrated with the thermal front, the finite element solution routine is not prone to result in unrealistic temperature values due to subsequent changes in α . Therefore, the value of α at the highest temperature of the region penetrated during a given Δt is the controlling parameter. Usually this controlling temperature is much lower than the maximum value.

Based on $k = 3.98 \text{ W/m}\cdot\text{K}$ and $\Delta x = 0.625 \text{ mm}$ Eq. (9) results in $0.07 < \Delta t < 0.21$ sec. The highest possible value of thermal conductivity (at $T = 3600 \text{ K}$) is $11.18 \text{ W/m}\cdot\text{K}$. The allowable Δt range corresponding to this k value is $0.025 < \Delta t < 0.075$ sec. As discussed earlier the controlling temperature is indeed much smaller than the maximum value (3600K). Therefore, $\Delta t < 0.075$ sec, is not an accurate estimation of the upper limit on Δt . Thus, the variable property test problem solution is obtained for $\Delta x = 0.625 \text{ mm}$ and $\Delta t = 0.1$ sec. (same as previous cases), and the results are tabulated in Table 4 along with SINDA-87 prediction.

The maximum variation between FAHT and SINDA-87 results is less than 0.8%. Thus, it can be stated with confidence that FAHT's variable property routine is reliable and accurate.

Table 4. Comparison of FAHT and SINDA - 87 Temperature predictions, $T(x,t) - T_i$, at Time = 2 seconds (Variable Property Verification).

| Code | x = 0 mm | 0.625 | 1.25 | 1.875 | 2.5 |
|----------|----------|-------|------|-------|------|
| FAHT | 2691 | 2341 | 1997 | 1667 | 1362 |
| SINDA-87 | 2705 | 2357 | 2012 | 1371 | 1680 |

- Test problem with $T_{\text{gas}} = 3600 \text{ K}$, $\varepsilon = 0.8$
- Thermal conductivity variable, $k = 3.98 + 0.002 T$
constant density and specific heat
- 320 elements, $\Delta t = 0.1 \text{ sec}$

III.4 Application to MNASA Nozzle

The variable property and nonlinear boundary condition routines of FAHT have been verified. Moreover, a procedure is proposed for obtaining a realistic transient solution from FAHT. It is further shown that with mesh refinement the procedure will converge to an accurate solution.

In this section, a course mesh model of MNASA nozzle will be used to obtain the temperature solution for variable property case with convection and radiation boundary condition. Since the results cannot be compared with any reliable solution, no attempts will be made at mesh refinement for obtaining an accurate solution. The course mesh model of MNASA nozzle along with the description of its various materials is depicted in Fig. 5.

The largest element size in the radial direction along the exposed surface to the thermal load is 0.547 in. Thermal diffusivity of all the materials (i.e., carbon phenolic, glass phenolic, silica phenolic, NBR rubber and steel) maybe relevant in the calculation of the allowable time step via Eq. (9). If the transient time is such that the thermal front reaches an interior material, then α of that region should be considered. Therefore, each material has its own restriction on the allowable time step. Moreover, the element size in the direction of heat flow may change from



GREEN - 0 DEG. CARBON PHEN.
 DK. BLUE - 90 DEG. "
 LT. BLUE - 60 DEG. "
 BLACK - 15 DEG. "
 YELLOW - 8 DEG. SILICA PHEN.
 LAVENDER - -15 DEG. GLASS PHEN.
 RED - NBR (RUBBER)
 PINK - STEEL

Figure 5. Coarse Mesh Model of MNASA Nozzle

material to material as well as within a given region. Variation of α with temperature is another factor which complicates the selection of proper time step. It is not in the scope of this study to calculate all the potential applicable ranges for the allowable time step. Therefore, the allowable time ranges for carbon phenolic and glass phenolic regions based on α values at about 1000°R and $\Delta x = 0.547$ in are calculated and presented. Δt range based on Eq. (9):

Carbon Phenolic: $90 < \Delta t < 270$ sec; Glass phenolic : $770 < \Delta t < 2300$ sec.

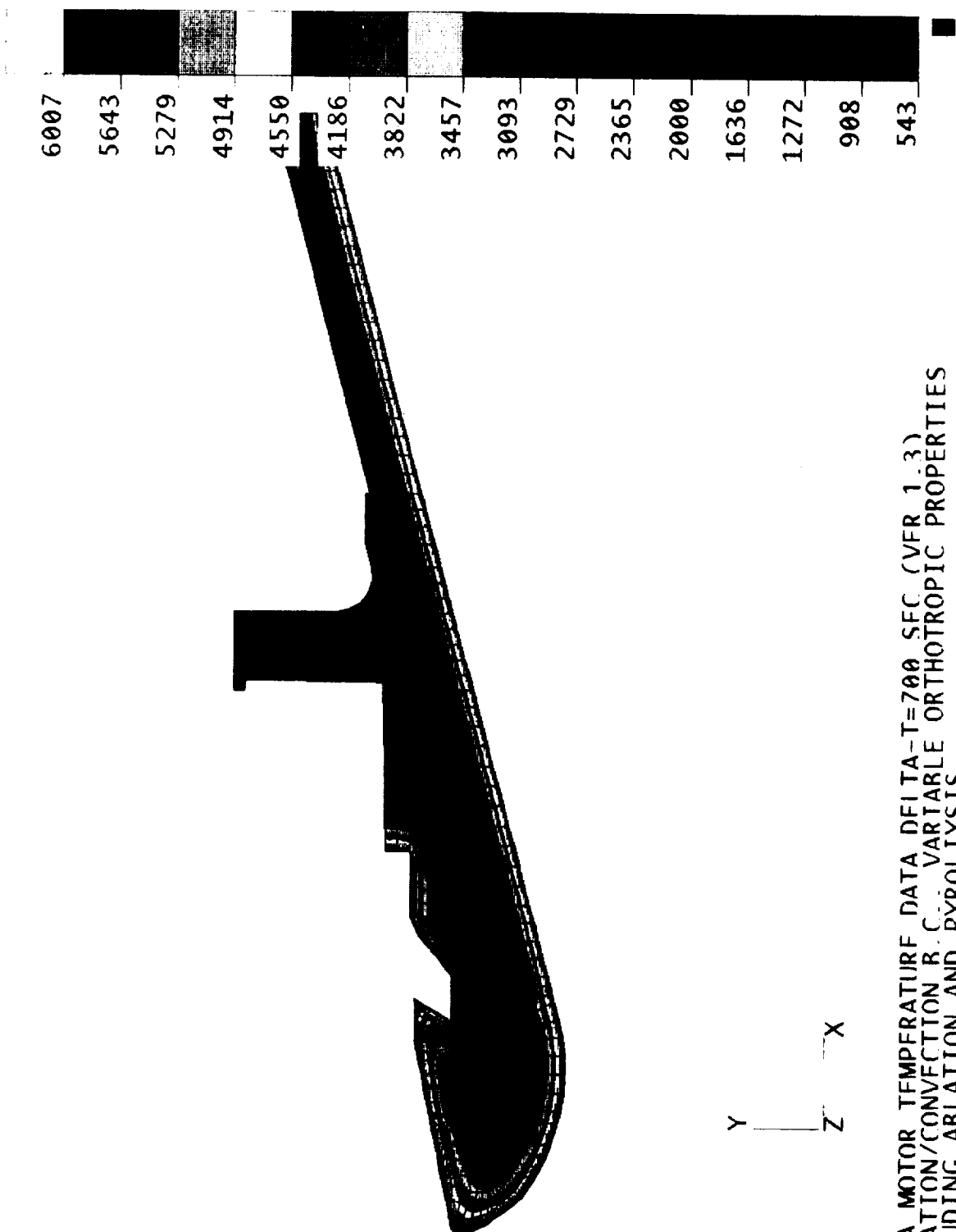
$$\alpha = 1.1 \times 10^{-3} \text{ in}^2/\text{sec};$$

$$\alpha = 1.3 \times 10^{-4} \text{ in}^2/\text{sec}$$

The criterion for carbon phenolic indicates that $\Delta t > 90$ sec. However, an estimate of location of the thermal front should be obtained to see if the glass phenolic region will be effected for time > 90 sec. The estimated penetration depth for $\alpha = 1.1 \times 10^{-3} \text{ in}^2/\text{sec}$ (carbon phenolic) and $\Delta t = 120$ sec is 1.26 in. It should be emphasized that $\delta = 1.26$ in is an estimate of the location of the thermal front. This calculation shows that the thermal front at time = 120 sec will be very close to the glass phenolic region. Therefore, the thermal diffusivity of this region may be relevant.

A FAHT run for the model with $\Delta t = 120$ sec resulted in a number of temperatures below the initial condition value. This indicates that the thermal front does indeed reach the glass phenolic region and the Δt restriction for this region should be considered ($770 < \Delta t < 2300$ sec). It should be added that the Δt restriction of this region is an estimate based on element thickness of 0.547 in and α at 1000°R. The actual element thickness in this region is less than 0.547 in, and a $\Delta t < 770$ sec will be acceptable. As stated earlier, the objective is to show the details of the procedure for Δt selection rather than tedious calculation.

FAHT's predicted temperature field for the coarse mesh model of MNASA nozzle with $\Delta t = 700$ sec after one time step is shown in Fig. 6. The predicted temperature field seems reasonable. In absence of a reliable solution to compare with no other conclusion can be drawn. The maximum predicted temperature at one node is 6007°F which is greater than $T_g = 6000^\circ\text{R}$. This is obviously an error. This error may be due to the input mesh geometry. Detail study of the mesh has revealed that in some regions the nodes of adjacent elements do not coincide. Moreover, there are elements which are triangular elements with four distinct nodes. FAHT can not account for traingular elements when the third and fourth nodes do not coincide. Unfortunately, the limited duration of this project did not allow for mesh correction and further investigation of the source of this error.



MNASE MOTOR TEMPERATURE DATA DF1TA-T=700 SEC (VFR 1.3)
 RADIATION/CONVECTION R.C. VARIABLE ORTHOTROPIC PROPERTIES
 EXCLUDING ABLATION AND PYROLYSIS

Figure 6. FAHT's Temperature Predictions at 700 sec with $T_i = 5300^{\circ}\text{R}$, $T_{\text{gas}} = 6000^{\circ}\text{R}$.

IV. CONCLUSIONS AND RECOMMENDATIONS

IV.1 Conclusions

The heat transfer module of FANTASTIC code (FAHT) is studied and evaluated to the extend possible during the ten weeks duration of this project. The conclusions of this work are:

- It is established that with improper choice of element size and time step FAHT's temperature prediction at some nodes, will be below the initial condition value. The source of this unrealistic temperature prediction is identified and a procedure is proposed for avoiding this phenomenon. It is further shown that the proposed procedure will converge to an accurate prediction upon mesh refinement.
- Radiation boundary condition solution routine of FAHT is verified.
- Variable property solution routine of FAHT is verified.
- Verification of the ability of FAHT to model convection heat transfer in a porous domain, independent of pyrolysis process, is not possible.
- FAHT users are advised to bypass the transient logic of FAHT by specifying a fixed time step based on the proposed criteria.
- Experienced and dedicated personnel working as a team are required for successful usage of FANTASTIC Code.
- The temperature field solution will have some errors due to lack of explicit treatment of the convection term.
- The pore pressure equation, as given by Eq. (3) is nonlinear. This equation, however, is treated as a linear equation in FAHT. Therefore, the pore pressure solution will not be accurate, which will result in an inaccurate velocity solution. The inaccuracy associated with the velocity solution, in turn, will increase the error in the temperature solution.
- The flow of pyrolysis gases through the char zone are modeled as a non-reacting low (frozen). Therefore, the endothermic reactions which take place in this zone can not be accounted for. Furthermore, the changes in the porosity and permeability in this zone cannot be calculated and accounted for.
- The permeability of the material is assumed to have the same value in the virgin, decomposition and char zones. As mentioned earlier, the permeability is changing rapidly with time in the decomposition zone. Nonetheless, FAHT can not account for this variation.

- There are no provisions for accounting for the initial porosity of the virgin material.
- The momentum equation is based on the Darcy law. However, it is known (NASA CR-1903, 1971) that the inertial effects play an important role due to relatively high mass fluxes of the degradation products. An accurate modeling of the momentum equation requires the inclusion of the Forchheimer term. Another motivation for the use of Forchheimer-extended Darcy equation of motion for flow through porous media is the following. One of the objectives of the exploratory test program of the Solid Propulsion Integrity Program (SPIP) is to provide empirical relations for permeability of various candidate materials. There may be cases where the permeability should be determined via the Forchheimer-extended Darcy equation. In that case we do not have any analysis tool that can properly use the permeability data.

IV.2 Recommendations

The recommendations of this study have two objectives. First, the issues which should be worked in order to get FAHT in an operational status. The second objective has a long term view of the required capabilities for accurate analysis of charring-decomposing ablator materials including future candidate composites.

Immediate issues which should be addressed in order to get FAHT in an operational status are:

- Fixing of the identified bugs.
- Details of the modeling and programming of the convection heat transfer of the pyrolysis gas as well as the mass diffusion equation should be provided by FaAA for accuracy analysis.
- Verification of pyrolysis modeling (without ablation) through a comparison of a one-dimensional problem with CMA.
- Verification of FAHT's ability to model the moving ablating surface through a comparison of a one-dimensional problem with CMA.
- Test run of an MNASA motor model with a refined mesh.

The motivation for recommending a long-term plan of work is as follows. The problem of analysis of a charring-decomposing material with an ablating surface is very complex and difficult. Experimental verification of any code is difficult, expensive and at best will provide a very rough, within the range, comparison. At the present time we do not have a "research" tool which models the energy and pore pressure equations accurately without any expedient simplifications for ease of programming. Moreover, we do not have a tool which models a dynamic permeability and can account for reactions between the pyrolysis gases and the char zone. Additional concern is that we do not have a code whose momentum equation includes the inertial effects which can play an important role when the mass fluxes are relatively high. In short, we do not have a research tool that includes all the known effects. Therefore, the research, development, design and testing verification can not proceed in a systematic manner. A research code, not a user friendly code or necessarily computationally efficient code, is needed to approach the problem in a systematic fashion. In that case, we can establish and distinguish primary, secondary and tertiary effects. This research code should have provisions to accommodate the data about the behavior of new candidate materials as becomes available. Concurrent with development of this research code, experimental work must proceed to provide extensive data about thermophysical properties, permeability and the possible reactions that take place in the char zone.

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